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Surface Roughness Effects in Low Reynolds Number Channel Flows (Preprint)

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Abstract. Rarefied helium and nitrogen flow expanding into vacuum through 150μm high and 1.5 cm long channels is studied experimentally and numerically with the DSMC method. Different types of channel walls are examined, both polished and rough with well characterized roughness shaped as triangles and rectangles. The pressure varies from 200 to 13,000 Pa, with the gas mean free path being both much larger and much smaller than the roughness size of about 20μm. A conical surface roughness model applicable for the DSMC method is proposed. An expression relating this model to the Cercignani-Lampis scattering model is derived. Good agreement between the numerical and experimental results is observed for the rough walled channel.

Keywords: Surface roughness, rarefied gas flows, DSMC, mass flow measurements
PACS: 51.10.+y, 51.90.+r

INTRODUCTION

Surface roughness plays a significant role for a number of gas dynamic problems. Traditionally, the surface structure and roughness are important in low-speed microflows, where the surface-to-volume ratio is high and surface effects dominate the gas flow. One example is the contribution of surface roughness to the resistance of gas channel flows currently drawing significant interest from researchers [1]. In addition to low-speed gas flows, the surface roughness effect may be significant in a number of high-speed flows [2]. This is true not only for micro-scale high-speed flows, where the roughness characteristic size becomes comparable to the flow dimensions, but also for large scale flows, where the local rarefaction may be observed even in flows that are generally in continuum regime.

Numerical modeling of the surface roughness effects in rarefied gas flows encounters a number of problems, from the difficulty of accurate description of complex surface shapes and roughness patterns, to the uncertainties of numerical validation. The description of rough surfaces has been approached before, both using simplified models such as cone models [3, 4] as well as more sophisticated models such as fractals models [5, 6]. The conical roughness model [4] where the surface is represented by a number of virtual cones has been applied to model the flow conductance in channels with the direct simulation Monte Carlo method, and the results were compared with available experimental data. It is not clear however whether the model satisfies detailed balance principle at equilibrium. The fractal model [6] is much more general, although still needs to be validated for rarefied gas flows.

The problems of validation of numerical models of surface roughness are related not only to the challenges of reliable and accurate measurement of low speed rarefied flows, but also to the physical complexities associated with gas-surface collisions. The related experimental studies of surface roughness are the work by Sugiyama et al [7] where triangular roughness in channel flows was studied numerically and experimentally for large Knudsen numbers and by Turner et al [8] where the surface roughness was found to have small effect on gas pressures inside a channel for several pressure ratios.

The accommodation of gas molecules is different for different angles of incidence [9], gas temperatures, surface temperatures, surface material and cleanliness. An additional process that may affect the flow in long microchannels is the variation of accommodation with local gas pressure via coverage dependence. In most cases, the probability of surface sticking/adsorption (and resulting near-complete thermal accommodation) decreases as the availability of surface sites decreases. Lundstrom [10] observed the surprising result that Knudsen flow diffusion increased with backing pressure. This was hypothesized to be due to the variation in sticking with local gas density and a tendency of molecules to scatter more specularly off adsorbed molecules than off the bare wall.

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Additional complexity of the surface roughness modeling is associated with the fact that in gaseous microflows, where the pressures are typically on the order of one atmosphere, and the mean free path is several tens of nanometers, the Knudsen number based on the characteristic roughness size varies significantly. The main objective of this paper is the numerical and experimental study of the surface roughness effects in the two-dimensional channel flow with well characterized surface roughness in the regimes from near free molecular to near continuum based on the roughness size. A simple model of the surface roughness that maintains the detailed balance and is applicable to the direct simulation Monte Carlo method is developed and its connection to the Cercignani-Lampis scattering kernel is established. The model is used in the DSMC computations of a helium flow through a long channel expanding into vacuum. The companion experimental study includes both nitrogen and helium mass flow measurements in the pressure range from about 1 Torr to 100 Torr for a channel thickness of 150μm.

CONICAL MODEL OF SURFACE ROUGHNESS FOR PARTICLE APPROACHES

The process of collisions of molecules with a rough surface can be split into the following stages: a molecule hits the wall at a certain point, experiences one or several collisions with the surface, and then leaves the wall. When the characteristic size of the roughness is significantly less that the gas mean free path, no intermolecular collisions take place during the second stage. The time for this stage is in this case much smaller than the mean collision time, and the distance traveled along the wall is on the order of the roughness size. Therefore, this time and distance can be ignored, and it is sufficient to specify only the reflected velocity of the molecule. The following approach is proposed to calculate the velocity of the reflected molecule. The surface is presented as a number of virtual conical holes with a fixed opening angle β and a height h randomly scattered over the actual surface. The after-collision velocity is calculated through the following steps. First, the molecule is assumed to cross the base of the cone at a random point A, as shown in Fig. 1s. Then, its subsequent collision point B with the side of the cone is calculated, and reflected velocity according to the diffuse reflection law is selected. The process of finding collision points and selecting new velocities is repeated until the molecule leaves the surface, that is, exits the conical hole through the base. Note again, the reflection point is assumed to be the same as the initial approach point, therefore, the actual value of h is not important (for example, $h = 1$m can be used). In this algorithm, there are no uncertainties associated with the cut-off for very long traveling distances such as those in [3]. It can also be easily implemented in DSMC. With such a surface shape simplification, there is only one parameter, namely average surface slope, that is used.

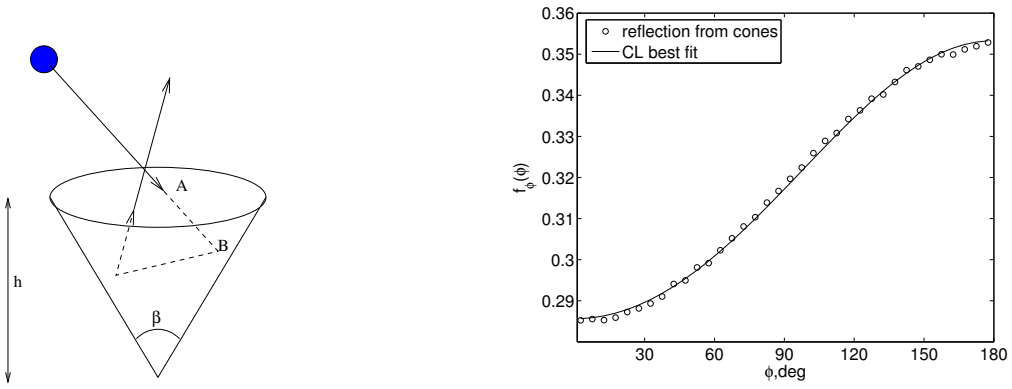

FIGURE 1. (a) Schematic of molecule reflection from the wall. (b) Distribution function of the angle between the reflected molecular velocity and flow direction, M=0.3, $\beta = 66^o$.

To study the influence of the rough wall on the flow properties, let us now examine how the velocity distribution function of the incident molecules is transformed by collisions with the wall. In what follows, the velocity distribution function of the incoming molecules is assumed to be equilibrium at a flow velocity characterized by the Mach number M and directed along x axis, where the wall is assumed to lie in xy plane. The distribution function of the angle ϕ ($0 < \phi < \pi$) between the reflected tangential molecular velocity and flow direction obtained using the reflection algorithm described above is plotted in Fig. 1b (circles) for $\beta = 66^\circ$ and M=0.3. Note that the maximum of the distribution function corresponds to the direction opposite to the flow direction, which is reasonable for a rough surface that is generally expected to increase flow resistance.

Let us show that this distribution can be fitted by the distribution obtained with the Cercignani-Lampis (CL) [11],[12] transformation of incident velocities. The analytical form of the distribution function obtained by using CL transformation is derived as follows. In what follows, it is assumed that the temperatures of the gas and the wall are equal, and the velocities are normalized by $\sqrt{m/kT}$. Then, the distribution functions of x and y velocity components of incident molecules are

$$f_x^{\text{inc}}(v) = \frac{1}{\sqrt{2\pi}} \exp(-(v - M\sqrt{\gamma})^2/2) \text{ and } f_y^{\text{inc}}(v) = \frac{1}{\sqrt{2\pi}} \exp(-v^2/2), \tag{1}$$

respectively. After the CL transformation, the x component of the reflected velocity is equal to

$$v_x^{\text{refl}} = \frac{1-\alpha_t}{\sqrt{|1-\alpha_t|}} v_x^{\text{inc}} + v_x^{CL}, \tag{2}$$

where the distribution function of v_x^{CL} is given by

$$f_x^{CL}(v) = \frac{1}{\sqrt{2\pi(1-|1-\alpha_t|)}} \exp\left(-\frac{v^2}{2(1-|1-\alpha_t|)}\right). \tag{3}$$

Here, α_t is the CL parameter that corresponds to the tangential accommodation coefficient, $0 \leq \alpha_t \leq 2$. Note that v_x^{refl} is the sum of the two independent normally distributed variables, therefore, its distribution function can be written as

$$f(v_x^{\text{refl}}) = \frac{1}{2\pi} \exp\left(-\left(v_x^{\text{refl}} - M\sqrt{\gamma}\frac{1-\alpha_t}{\sqrt{|1-\alpha_t|}}\right)^2\right). \tag{4}$$

Similarly, it can be concluded that the distribution function of y velocity component does not change during CL transformation. Note that $\tan(\phi) = \frac{|v_y^{\text{refl}}|}{v_x^{\text{refl}}}$, so for $0 < \phi < \pi/2$ the distribution function of ϕ can be obtained with

$$f(\tan\phi) = \int_0^\infty u_x f_x^{\text{refl}}(u_x) f_y^{\text{refl}}(u_x \tan\phi) du_x \tag{5}$$

and for $\pi/2 < \phi < \pi$

$$f(\tan\phi) = -\int_{-\infty}^0 u_x f_x^{\text{refl}}(u_x) f_y^{\text{refl}}(u_x \tan\phi) du_x. \tag{6}$$

Finally, the reflected velocity distribution function

$$f_\phi(\phi) = 2f(\tan\phi)(1+\tan^2\phi) = \frac{\exp(-t^2)}{\pi} + \frac{t\cos\phi}{\sqrt{\pi}} \exp\left(-t^2\sin^2\phi\right)(1+\text{erf}(t\cos\phi)), \tag{7}$$

where $t = \frac{1-\alpha_t}{\sqrt{|1-\alpha_t|}} M\sqrt{\gamma}$.

Parameter α_t of the CL transformation can be found by least square fitting of ϕ distributions obtained using the reflection algorithm described in section to Eq.(7). Figure 1b shows such a fit. α_t is larger than 1, which means that the average tangential momentum of the reflected molecules points in the opposite direction with respect to the average tangential momentum of the incident molecules. $\alpha_t = 1$ corresponds to zero average momentum of reflected molecules, and the bigger the difference between α_t and 1, the bigger the average momentum of reflected molecules.

Figure 2a shows the values of α_t found by a least square fit for M=0.3 and different cone opening angles. As expected, α_t is maximum for some intermediate value of cone opening angle. A large opening angle essentially means that the surface is flat, so α_t tends to 1 in this case. Also, α_t decreases for small opening angles.

The value of α_t only weakly depends on Mach number, which is illustrated in Fig. 2b, where α_t is shown as a function of the Mach number for two different opening angles, $\beta = 120^o$ and $\beta = 66^o$ (the latter one is used in the

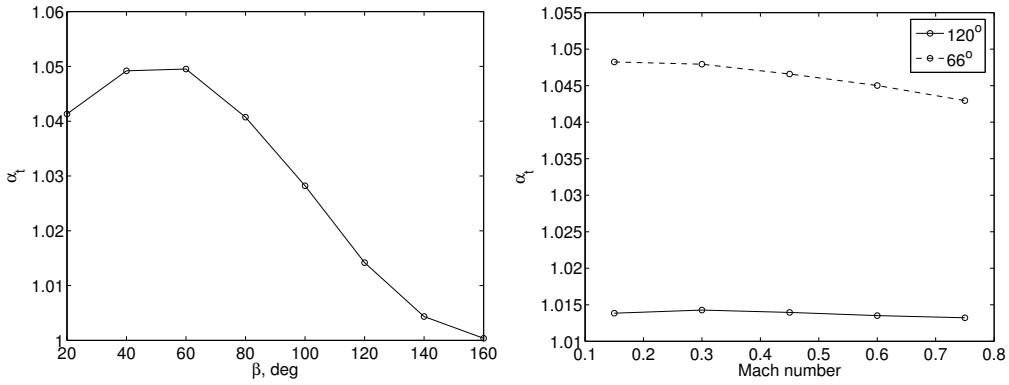

FIGURE 2. (a) α_t as a function of cone opening angle β, M=0.3 (b) α_t as a function of Mach number for two cone opening angles.

experiments). This fact facilitates the use of the CL model in DSMC simulations, since the value of α_t can be selected depending on the degree of roughness of the surface, and not on flow properties.

The verification of the rough surface model has been performed for a two-dimensional thermal bath test case, with the test gas being helium initially heated to 1000 K. The surface temperature was assumed constant at 300 K, and the conical roughness model was used with a cone angle of 45 deg. The temporal temperature relaxation inside the test box is illustrated in Fig. 3 for a cross section along the centerline. As particles collide with the surface, the temperature decreases from its initial value to the equilibrium value of 300 K. This test case shows that the detailed balance is maintained in the conical roughness model, and in may be used in DSMC modeling of gas flows. The present numerical and experimental study concentrates on rarefied gas flows though a long channel into vacuum, and the flow conditions and setup are given in the next sections.

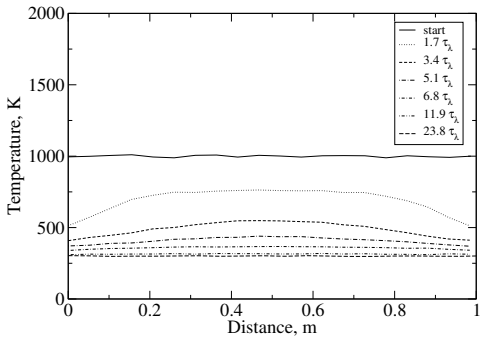

FIGURE 3. Temporal relaxation of gas temperature in a 300 K box. Time is in mean collision times τ_λ at 1000 K.

EXPERIMENTAL SETUP AND CONDITIONS

A flat polished surface, a regular triangular groove, and a regular square groove texture was tested during this experiment. The details of tested geometries are summarized in Fig. 4. The 2 cm by 1.5 cm silicon texture inserts were fabricated through standard MEMS processes. At the entrance and exit of the channel is a shelf between 1 and 5 features long; with approximately 800 features down the length of the channel, the influence of this shelf is negligible. The inserts were placed in an aluminum holder and Teflon sheet assembly. The spacing between the two center Teflon sheets determines the width of the channel while the thickness of these sheets determines the height. The design dimensions for the channel are 1 cm wide, 150 microns high, and 1.5 cm long (the later being the flow direction). This

assembly was then placed in one wall of a 3550 cm^3 plenum, which acted as a stagnation chamber. Two inlet ports and three pressure ports also penetrate the wall of the plenum.

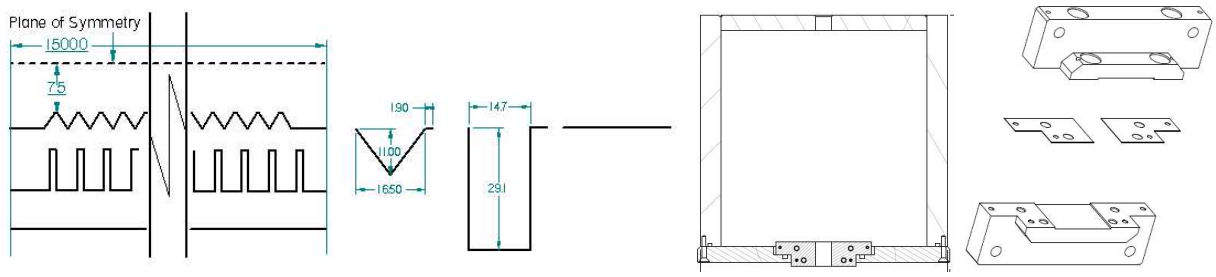

FIGURE 4. Experimental specifications and setup.

The entire setup was then placed in the Collaborative High Altitude Flow Facility (CHAFF) at the University of Southern California (USC) Chamber IV. The chamber is a 3 m diameter by 6 m long high vacuum chamber pumped by a 1 m diameter diffusion pump capable of 25,000 L/s for nitrogen and 42,000 L/s for helium. The ultimate background pressure of the chamber is 10^{-6} Torr with working pressures as high as 10^{-4} Torr. The stagnation pressure in the plenum was tested between 1 and 100 Torr for both helium and nitrogen. Before and immediately after testing, the assembly was analyzed in a Cambridge 360 Scanning Electron Microscope (SEM). The SEM images of three surfaces under consideration are presented in Fig. 5. The assembly was measured to find the exact channel height with an accuracy of 2 microns. A jeweler's microscope with an accuracy of 25.4 microns was used to find the channel width. The accuracy of the groove dimensions was 0.2 microns.

The mass flow of the test gas was monitored until the pressure in the plenum became constant. The data was recorded and the mass flow adjusted to the next data point. This was conducted for both helium and nitrogen using Omega 1000, 100, 10, and 5 SCCM mass flow meters and MKS 100, 10, 1, and .2 Torr Baratrons.

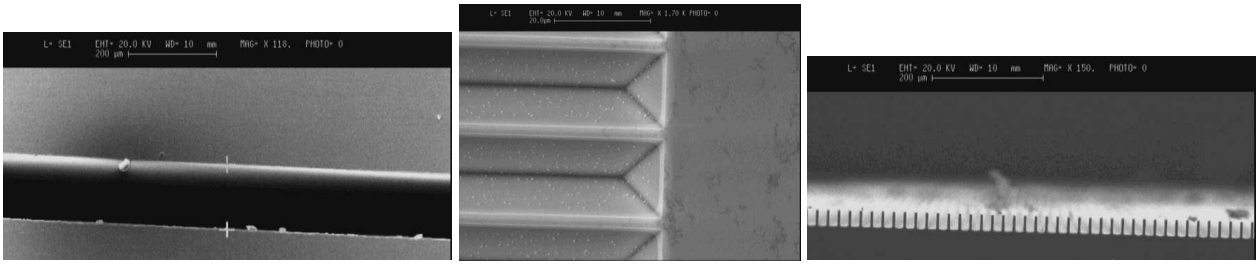

FIGURE 5. SEM images of a polished channel (left), triangular grooves (center), and rectangular grooves (right).

NUMERICAL APPROACH

The DSMC-based software system SMILE [13] was used in all DSMC computations. A 2D capability of SMILE was used in this work. The majorant frequency scheme was used to calculate intermolecular interactions. The intermolecular potential was assumed to be a variable hard sphere. The conical roughness model has been implemented in SMILE for the gas-surface interactions, and the following four surfaces were used in the computations: (i) fully diffuse flat surface with complete energy and momentum accommodation; (ii) flat surface with the conical roughness and diffuse accommodation on cone sides and an opening angle of 66° that corresponds to the experimental conditions; (iii) CL model with a tangential momentum accommodation coefficient of 1.045 to approximate (ii); (iv) a diffuse surface that consists of about 800 triangles and approximate the actual experimental shape.

The channel height and length were 150 μm and 1.5 cm, respectively. Helium was used as the test gas, and the chamber pressure varied from 200 Pa to 13,000 Pa. The Knudsen number based on the stagnation conditions and the feature size of about 20μm ranged from about 5 down to 0.1. The convergence study computations were performed for 6000 Pa and two inflow boundaries, the first extending 1700μm from the channel entrance and 1700μm from the symmetry plane, the other 850 by 850μm, respectively. The Maxwellian distribution function with zero flow velocity was assumed at these boundaries; no impact of the boundary location on the results was found. The larger domain was

used in all subsequent computations, with the number of molecules ranging from about 1.6 million for the smaller pressures to about 10 million for the larger ones.

RESULTS AND DISCUSSION

Consider first the results of the DSMC modeling of a helium flow inside a two-dimensional channel. The distribution of pressure and Mach number along the channel is shown in Fig. 6a for the smallest and the largest pressures under consideration and a fully diffuse flat surface. For the stagnation pressure of 200 Pa, the local Knudsen number based on the channel height increases from about 1 to 100, and for this essentially free molecular flow the gas pressure decreases linearly from the stagnation value, P_0, to about $0.01P_0$ at the channel exit. The Mach number is below 0.05 for most of the channel, except for the vicinity of the exit where it increases to 1. As expected, the Mach number is higher for the larger pressure, but still mostly less than 0.1.

The calculated mass flow as a function of stagnation pressure is given in Fig. 6b for four surface models under consideration. Several conclusions can be drawn from these results. First, the surface roughness results in decreasing the mass flow by about 30% for 200 Pa, and then the difference decreases to about 6% for 10,000 Pa. Second, the CL model with $\alpha_t = 1.045$ agrees with the conical roughness model within two percent for lower pressures and less than one percent for higher pressures. Finally, the results for the two surface roughness models are in good agreement with the results for the triangulated surface, thus providing additional verification for the roughness models.

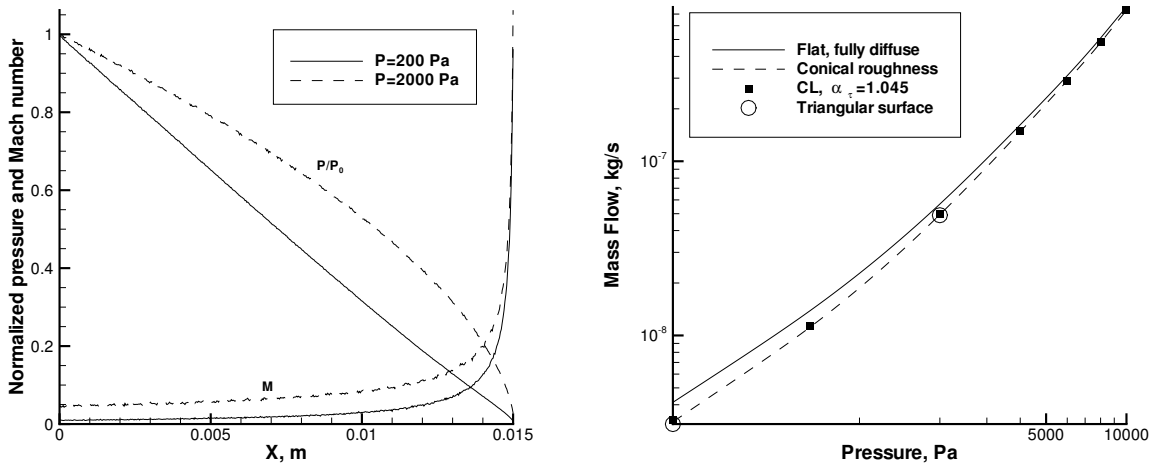

FIGURE 6. (a) Pressure normalized by the stagnation value and Mach number profiles along the channel centerline for two stagnation pressures. (b) Computed mass flow for different surface models.

The experimental results for three surfaces under consideration are presented in Fig. 7 for two gases. The results provide evidence for significant reduction in mass flow for rough surface channels both for helium and nitrogen. This result may appear contradicting to the conclusions of [8], but it may be explained by much larger (flatter) roughness angles used in [8] than that examined in this work. Although the impact of surface roughness at each given pressure is larger for helium than for nitrogen, it is similar if mass flow is plotted as a function of Knudsen number. The rectangular grooves result in mass flows higher than those for triangles, especially for the nitrogen flow, where they are relatively close to the flat surface case.

Let us now compare the experimental and numerical results on helium mass flow for smooth and rough surfaces. There is a good agreement between the results, with the numerical values being within the experimental error bar, estimated at about 10% for 200 Pa and less than 2% for 10,000 Pa, based on standard deviation. The only exception is at high pressures for the flat surface, where the DSMC results are over 4% lower than the measured points. There are three effects that may cause the difference between the numerical and experimental results: the side walls (three-dimensionality), surface specularity, and surface absorption.

The absence of the side walls in DSMC may result in overprediction of the mass flow, especially for lower pressures [14]. This effect may also be responsible for a slight difference between the experiment and DSMC for the rough

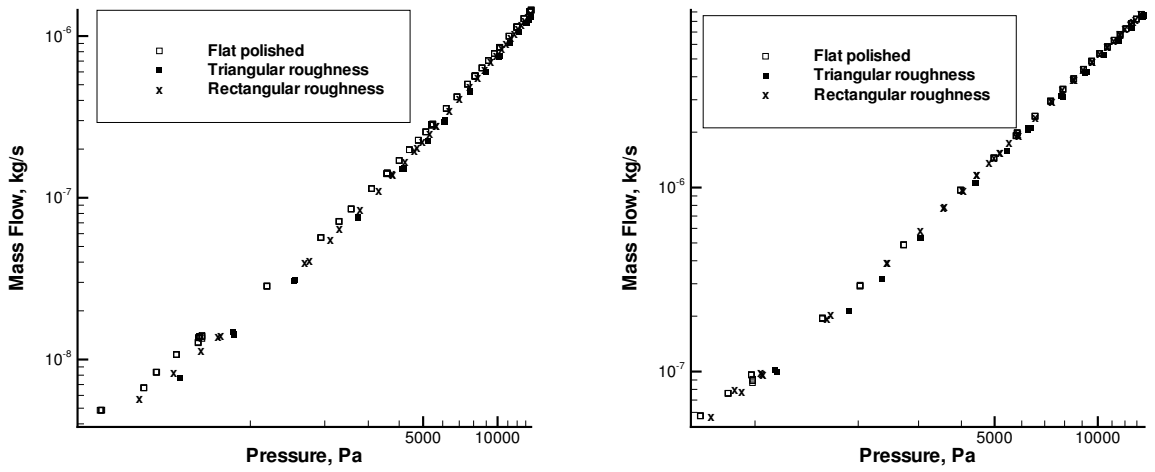

FIGURE 7. Measured mass flow through channel for helium (left) and nitrogen (right).

surface. On the other hand, a polished surface considered in the experiments may have some finite specularity not included in the numerical modeling, that would generally increase numerical values. The effect of surface absorption may increase with gas pressure. Although the magnitude of the effect of increasing adsorption leading to lower overall accommodation at higher pressure is difficult to estimate, it will lead to some increase in flow at higher pressure and could be another explanation of the data trend for the flat surface.

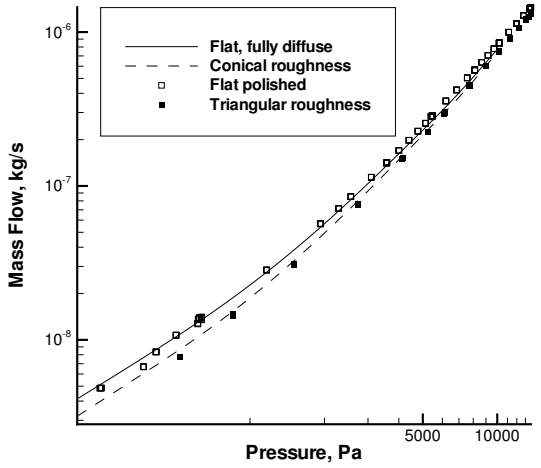

FIGURE 8. Comparison of computed (lines) and measured (symbols) mass flows for smooth and rough surfaces. Helium flow.

CONCLUSIONS

Rarefied gas flow expanding into vacuum through long channels with smooth or rough walls was examined experimentally and numerically with the DSMC method. Two gases, helium and nitrogen, were considered, with stagnation pressures varied from 200 Pa to 13,000 Pa for a 150μm high and 1.5 cm long channel. A conical surface roughness model applicable for the DSMC method was suggested and used in this work. An expression relating this model to

the Cercignani-Lampis scattering model is found, and reflected particle velocity distribution for the two models was shown to be close when the tangential accommodation coefficient is chosen appropriately. A significant impact of the surface roughness on mass flow through a channel was observed both experimentally and numerically. The mass flow in a rough channel is lower than that of a polished surface channel, with the difference amounting to 6% for larger pressures and 30% for smaller pressures. A good agreement between the numerical and experimental results is obtained for a rough surface channel, thus validating the conical roughness model. Experimental slope of the mass flow as a function of pressure is somewhat higher than that in DSMC, with the difference attributed to the combined effect of the flow three-dimensionality and surface coverage.

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